Databases and Software System for Thermodynamic Modeling in a Wide Range of Pressure and Temperature

V.E. Fortov, V.P. Efremov, V.S. Iorish,[C,S] V.S. Yungman, G.V. Belov, K.V. Khischenko, and P.R. Levashov
Institute for High Energy Densities of "IVTAN" Association of RAS
Izhorskaya 13/19, Moscow, 125412, Russia
iorish@tcras.chem.msu.su

S.A. Gubin and S.B. Victorov
Moscow Engineering Physics Institute, Kashirskoe Shosse 31
Moscow, 115409, Russia

I.V. Lomonosov
Institute of Problems of Chemical Physics of RAS, Chernogolovka
Moscow Region,142432, Russia

The collection of databases and software packages are designed to perform thermodynamic calculations of complex chemically reacting systems in a wide range of temperature and pressure. Standard state thermodynamic properties are taken from the IVTANTHERMO databank [1]. Original database of experimental data on shock adiabates [2] is used to construct realistic equations of state (EOS) for many solid substances. Several types of theoretical and semi-empirical EOS are applied for gases, liquids, and fluids [3]. The software package makes it possible to model such processes as shock compression, isentropic expansion, detonation of explosives, and other cases where it is difficult, or practically impossible to measure thermodynamic properties and compositions.

[1] G.V.Belov, V.S. Iorish, and V.S.Yungman, *Calphad*, **23**, 173 (1999).
[2] I.V. Lomonosov, A.V. Bushman, V.E. Fortov, and K.V. Khishchenko, "Caloric equations of state of structural material", in *High Pressure Science and Technology–1993*, New-York: AIP Press, 133-136 (1994).
[3] S.B. Victorov, S.A. Gubin, and I.V. Maklashova, *Shock Waves*, **11**, 105 (2001).